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Time Series Forecasting of Methane Concentrations in the Surface Layer of Atmospheric Air in Arctic Region

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Abstract. Time series forecasting is relevant in many fields of human activity. In particular, when studying the processes associated with global warming, such forecasts are very important. The present study used data of the concentration of the greenhouse gases (methane) in the surface layer of atmospheric air on the Arctic island Belyi, Russia. For the work, the time interval of 170 hours (about a week) was chosen during the summer period, characterized by significant daily fluctuations of methane concentration. Models based on artificial neural networks (ANN) such as Nonlinear Autoregressive Neural Network with an External Input (NARX), Elman Neural Network (ENN), and Multi-Layer Perceptron (MLP) were used for modelling. Methane concentrations corresponding to the first 150 hours of the interval used for ANN training, then the concentrations were predicted for the next 20 hours. The model based on the ANN type NARX showed the best accuracy.

INTRODUCTION

In many areas of human activity, the problems associated with forecasting time series are topical. In economics, medicine, ecology and nature management, and other areas, there is a need for forecasting time series. Such forecasts are very in demand in the studies concerning the problem of global warming, in particular, the dynamics of increasing concentrations of greenhouse gases. Climate change particularly affects the Arctic regions. So in recent years, the temperature in some areas of the Russian Arctic at 6-7 ° C exceeded the average long-term observations [1], [2]. For this phenomenon (rapid climate change in the Arctic) has its name - "Arctic reinforcement" [3].

Forecasting the dynamics of atmospheric air pollution is carried out both with the use of classical statistical approaches [4]-[6] and using models based on artificial neural networks, which have become particularly popular in recent years [7]-[11]. Among the many types of artificial neural networks with time series prediction problems, three types of networks are more suitable. These are MLP, Elman and NARX networks [12]-[21]. To obtain a prediction using a neural network, it is not necessary to isolate trend, random, and cyclic components in a time series. In the process of learning, these factors are determined by the neural network itself and taken into account in the construction of the prediction. The task is to obtain a qualitative forecast using the minimal input data.

To solve a specific problem, it is necessary to determine the structure of a particular network (the number of hidden layers, neurons in each layer, etc.). It is also very important to choose the correct learning algorithm.

MATERIALS AND METHODS

Measurements of greenhouse gases methane, carbon dioxide, carbon monoxide, and water vapor were made on the Arctic Island, Belyi, YNAO, Russia in summer 2015. The island is located in the Kara Sea 5-10 km north of the Yamal Peninsula (Fig.1). Concentration of greenhouse gases were measured by means of a cavity ring-down spectrometer Picarro G2401.

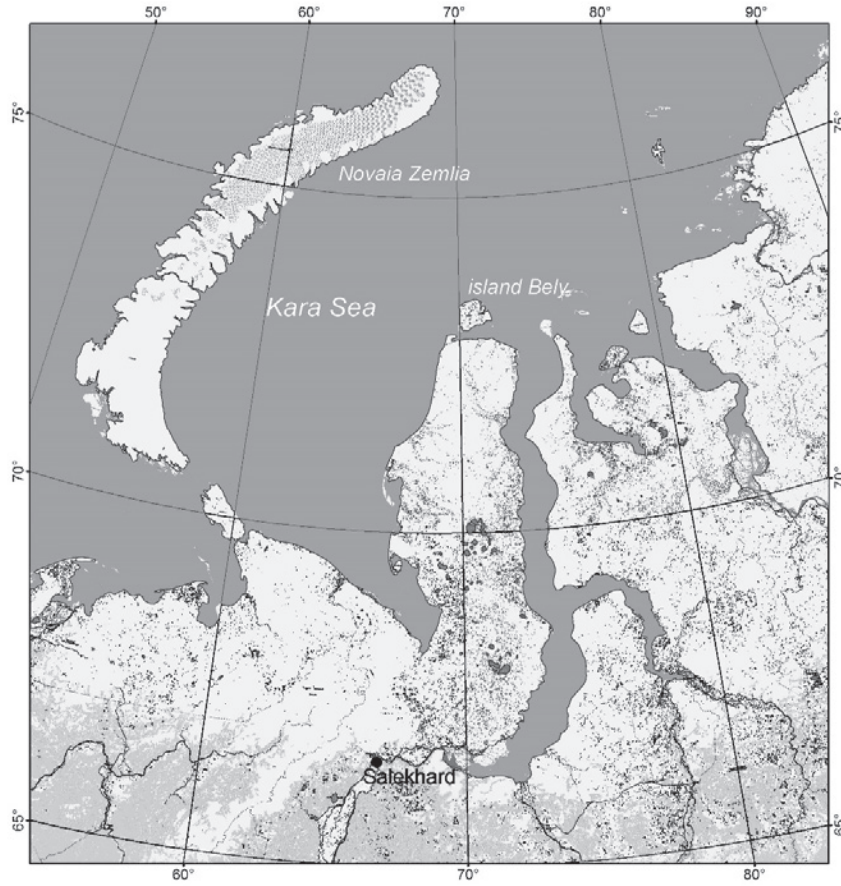


FIGURE 1. Place of measurements

In this work, time series of 170 intervals (hours) were chosen. For the prediction data on the methane content (ppm mole fraction) in the surface layer of atmospheric air were used. For modeling, the data was divided into two subsets. The first was used to train the network (adjusting the weights). Traditionally, this subset includes most of the test sample, which was 150 intervals in our case. The remaining 20 intervals formed a test subset. It was not used in the learning process of the neural network, and was used only to predict the values of the series.

To predict the time series, was selected the NARX network. It is a recurrent dynamic network with feedback consisting of several layers, it is based on the autoregressive model used to describe systems that have inertia. The predicted value depends on n previous output values and n previous values of the time series. As the input data, the time interval numbers were used in order, and as output - the value of the indicator (ppm mole fraction CH_4), corresponding to the time, applied to the input of the network. The standard NARX network is a two-layer network of reversed distribution. As a transfer function in the hidden layer, the sigmoidal function (1), and in the output layer - linear (2).

$$\varphi = \frac{1}{1+e^{-y}} \quad (1)$$

$$\varphi = y, \quad (2)$$

The standard NARX network is a two-layer network of reversed distribution. This network model uses delay lines with taps to store the previous values of $x(t)$ and $y(t)$. The output value of $y(t)$ is fed back to the network input with a delay, since $y(t)$ is a function that depends on the previous values: $y(t-1)$, $y(t-2)$, ..., $y(t-n)$.

The second ANN type Elman's neural network was used. Elman's network is one of the types of a recurrent network that is obtained from a multilayer perceptron by introducing feedbacks, with the connections not from the

output of the network but from the outputs of neurons of the inner layer. This allows to take into account the history of the observed processes and accumulate information to develop the correct prediction strategy. These networks are applicable to time series prediction problems, since their main feature is the memorization of sequences.

As third ANN type, a feed-forward MLP was used. MLP is direct propagation neural network. The input signal in such network propagates in a forward direction, from layer to layer. A MLP in a general representation consists of a plurality of input nodes that form an input layer of one or more hidden layers of computational neurons, and one output layer of neurons. The number of input and output elements in a multilayer perceptron is determined by the conditions of the problem. A MLP contains one or more layers of hidden neurons that are not part of the input or output of the network. These neurons allow the network to learn to solve complex problems, consistently extracting the most important characteristics from the input parameters. A MLP has a high degree of connectivity realized through synaptic connections. Changing the level of connectivity of the network requires changing the set of synaptic connections or their weighting factors. The combination of all these properties along with the ability to learn from own experience provides the computing power of a MLP.

The network structure was determined during computer simulation. The input layer of MLP was compiled with sampling points; the hidden layer consists of a several neurons, and the output layer represents the element concentration (ppm mole fraction CH_4) corresponding to the time.

The selection of the number of neurons in the hidden layer in NARX, Elman, and MLP was carried out by the lower root mean squared error (RMSE) (4). The number of neurons was varied from 5 to 25. Each network was trained 500 times and the best of them was selected.

Indices MAE (3), RMSE (4), root mean squared relative error (RMSRE) (5), and normalized root mean squared error (NRMSE) (6) was verified the predictive accuracy of each selected approach between the prediction and raw data from the training data set.

$$MAE = \frac{\sum_{i=1}^n |z_{mod}(x_i) - z(x_i)|}{n}, \quad (3)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (z_{mod}(x_i) - z(x_i))^2}{n}}, \quad (4)$$

$$RMSRE = \sqrt{\frac{1}{n} \sum_{i=1}^n \left(\frac{z_{mod}(x_i) - z(x_i)}{x_i} \right)^2} \quad (5)$$

$$NRMSE = 1 - \sqrt{\frac{\sum (z_{mod}(x_i) - z(x_i))^2 / n}{\sum (z_{mod}(x_i) - \bar{z})^2 / n}} \quad (6)$$

where $z_{mod}(x_i)$ is a predicted concentration, $z(x_i)$ is a measured concentration, \bar{z} is a mean concentration, and n is a number of points.

RESULTS AND DISCUSSION

For all types of ANNs the Levenberg-Marquardt training algorithm was used [14]. The final neuron number in the hidden layer was 20 for NARX, Elman and MLP networks.

TABLE 1. Accuracy assessment indices of the CH_4 concentration

Method	MAE, ppm	RMSE, ppm	RMSRE, ppm	NRMSE, ppm
Training interval				
MLP	0.004	0.006	0.003	0.542
Elman	0.005	0.008	0.004	0.410
NARX	0.005	0.008	0.004	0.389
Test interval				
MLP	0.012	0.014	0.007	0.007
Elman	0.011	0.013	0.007	0.117
NARX	0.007	0.009	0.005	0.359

Table 1 shows the parameters used to compare the performance of the different methods (the best values demonstrated by NARX for the test interval are in **bold**). Taking into account all indices, the NARX network showed better forecast accuracy. In addition, the model showed approximately the same result for the entire predicted time

interval. The MLP network showed the acceptable accuracy for a time interval of about 10 hours (20% of the entire test interval), but then predicted an average value (Fig. 2).

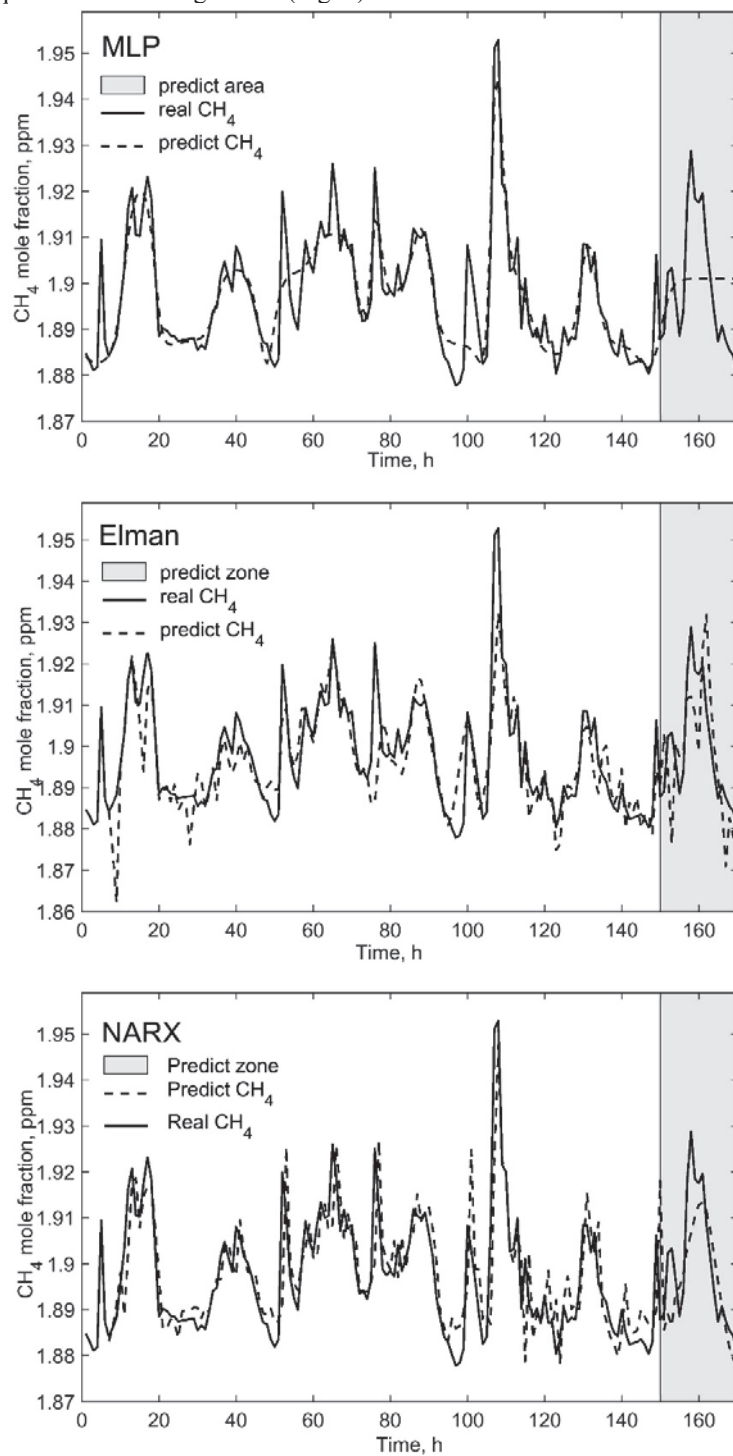


FIGURE2. Comparison of different prediction approaches.

CONCLUSION

The paper presents a comparison of the models based on ANN type Multilayer Perceptron, Elman network, and NARX for time series prediction. For the study, concentrations of one of the main greenhouse gases, methane, were taken. The data were obtained by monitoring greenhouse gases on the Arctic island Belyi, YNAO, Russia. For ANN training, the results were used for a time interval of 150 hours, the forecast followed for the next 20-hour interval. The minimal error for training was shown by the Elman network and MLP, but the NARX network provided the best forecast. The low accuracy of the MLP forecast is due to the lack of feedback in the network structure, which caused a short forecasting horizon. Nevertheless, for problems requiring a short horizon, network predictions based on MLP may be applicable.

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